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APPENDIX A

ALUMINUM CHLORIDE ROBUST SUMMARIES

6/8/2004

I U C L I D

Data Set

Existing Chemical : ID: 57-11-4
EINECS Name : stearic acid
EC No. : 200-313-4
Molecular Formula : C18H36O2

Producer related part
Company : Epona Associates, LLC
Creation date : 04.12.2003

Substance related part
Company : Epona Associates, LLC
Creation date : 04.12.2003

Status :
Memo : SOCMA MCC

Printing date : 05.12.2003
Revision date :
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Number of pages : 22

Chapter (profile) : Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile) : Reliability: without reliability, 1, 2, 3, 4
Flags (profile) : Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE),
Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 APPLICANT AND COMPANY INFORMATION

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

1.1.0 SUBSTANCE IDENTIFICATION

1.1.1 GENERAL SUBSTANCE INFORMATION

Purity type	:	
Substance type	:	organic
Physical status	:	solid
Purity	:	-
Colour	:	Colorless, waxy solid
Odour	:	SLIGHT TALLOW-LIKE ODOR
Source	:	Epona Associates, LLC
Reliability	:	(2) valid with restrictions
		Information taken from a peer-reviewed publication.

04.12.2003

(5)

04.12.2003

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADE NAMES

1.3 IMPURITIES

1.4 ADDITIVES

1.5 TOTAL QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.6.3 PACKAGING

1.7 USE PATTERN

1.7.1 DETAILED USE PATTERN

1.7.2 METHODS OF MANUFACTURE

1.8 REGULATORY MEASURES

Type of measure :
Legal basis : other: Generally Recognized as Safe
Remark : [Code of Federal Regulations]
[Title 21, Volume 3]
[Revised as of April 1, 2003]
From the U.S. Government Printing Office via GPO Access
[CITE: 21CFR184.1090]

TITLE 21--FOOD AND DRUGS

CHAPTER I--FOOD AND DRUG ADMINISTRATION
DEPARTMENT OF HEALTH AND HUMAN SERVICES
PART 184--DIRECT FOOD SUBSTANCES AFFIRMED AS GENERALLY
RECOGNIZED AS SAFE

Subpart B--Listing of Specific Substances Affirmed as GRAS

Sec. 184.1090 Stearic acid.

(a) Stearic acid (C₁₆H₃₆O₂, CAS Reg. No. 57-11-4) is a white to yellowish white solid. It occurs naturally as a glyceride in tallow and other animal or vegetable fats and oils and is a principal constituent of most commercially hydrogenated fats. It is produced commercially from hydrolyzed tallow derived from edible sources or from hydrolyzed, completely hydrogenated vegetable oil derived from edible sources.

(b) The ingredient meets the specifications of the Food Chemicals Codex, 3d Ed. (1981), p. 313, which is incorporated by reference, and the requirements of Sec. 172.860(b)(2) of this chapter. Copies of the Food Chemicals Codex are available from the National Academy Press, 2101 Constitution Ave. NW., Washington, DC 20418, or available for inspection at the Office of the Federal Register, 800 North Capitol Street, NW., suite 700, Washington, DC 20408.

(c) In accordance with Sec. 184.1(b)(1), the ingredient is used in food with no limitation other than current good manufacturing practice. The affirmation of this ingredient as generally recognized as safe (GRAS) as a direct human food ingredient is based upon the following current good manufacturing practice conditions of use:

(1) The ingredient is used as a flavoring agent and adjuvant as

defined in Sec. 170.3(o)(12) of this chapter.

(2) The ingredient is used in foods at levels not to exceed current good manufacturing practice.

(d) Prior sanctions for this ingredient different from the uses established in this section do not exist or have been waived.

Reliability
05.12.2003

[48 FR 52445, Nov. 18, 1983, as amended at 50 FR 49536, Dec. 3, 1985]
: (1) valid without restriction

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

1.8.2 ACCEPTABLE RESIDUES LEVELS

1.8.3 WATER POLLUTION

1.8.4 MAJOR ACCIDENT HAZARDS

1.8.5 AIR POLLUTION

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1.9.2 COMPONENTS

1.10 SOURCE OF EXPOSURE

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

1.13 REVIEWS

2.1 MELTING POINT

Value : = 69 - 70 °C
Sublimation :
Method :
Year : 1982
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Source : Epona Associates, LLC
Reliability : (2) valid with restrictions
Information taken from a peer-reviewed publication.

Flag : Critical study for SIDS endpoint
04.12.2003

(16)

2.2 BOILING POINT

Value : = 383 - °C at 1013 hPa
Decomposition :
Method :
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Source : Epona Associates, LLC
Reliability : (2) valid with restrictions
Information taken from a peer-reviewed publication.

Flag : Critical study for SIDS endpoint
04.12.2003

(16)

2.3 DENSITY

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value : = 1.33 - hPa at 173.7 °C
Decomposition :
Method :
Year : 1969
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Source : Epona Associates, LLC
Reliability : (2) valid with restrictions
Information taken from a peer-reviewed publication.

Flag : Critical study for SIDS endpoint
04.12.2003

(15)

2.5 PARTITION COEFFICIENT

2. Physico-Chemical Data

Id 57-11-4

Date 05.12.2003

Partition coefficient : octanol-water
Log pow : = 8.42 - at °C
pH value : -
Method :
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Source : Epona Associates, LLC
Reliability : (2) valid with restrictions
Information taken from a peer-reviewed publication.
04.12.2003 (9)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in : Water
Value : = .568 - mg/l at 25 °C
pH value : -
concentration : at °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description :
Stable :
Deg. product :
Method : other: measured
Year : 1966
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Result : Water solubility = .0001 mg/L at 30 deg C
Reliability : (2) valid with restrictions
Information taken from a peer-reviewed publication.
05.12.2003 (12)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

2. Physico-Chemical Data

Id 57-11-4
Date 05.12.2003

2.13 VISCOSITY

2.14 ADDITIONAL REMARKS

3. Environmental Fate and Pathways

Id 57-11-4
Date 05.12.2003

3.1.1 PHOTODEGRADATION

Type : air
Light source :
Light spectrum : - nm
Relative intensity : - based on intensity of sunlight
DIRECT PHOTOLYSIS
Half-life t_{1/2} : = .5 - day(s)
Degradation : - % after
Quantum yield :
Deg. product :
Method : other (calculated)
Year : 2003
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Method : Estimated using AopWin v1.91
Result : Atmospheric Oxidation (25 deg C) [AopWin v1.91]:
Hydroxyl Radicals Reaction:
OVERALL OH Rate Constant = 22.4804 E-12 cm³/molecule-sec
Half-Life = 0.476 Days (12-hr day; 1.5E6 OH/cm³)
Half-Life = 5.710 Hrs
Ozone Reaction:
No Ozone Reaction Estimation

Source : Epona Associates, LLC
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
04.12.2003

Type : air
Light source :
Light spectrum : - nm
Relative intensity : - based on intensity of sunlight
DIRECT PHOTOLYSIS
Half-life t_{1/2} : = 17 - hour(s)
Degradation : - % after
Quantum yield :
Deg. product :
Method :
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Result : Vapor phase stearic acid is degraded in the atmosphere by reaction with photochemically-produced hydroxyl radicals with a half-life of about 17 hours.

Source : Epona Associates, LLC
Reliability : (2) valid with restrictions
Information taken from a peer-reviewed publication.

05.12.2003

(1) (3) (6) (10)

3.1.2 STABILITY IN WATER

3.1.3 STABILITY IN SOIL

3. Environmental Fate and Pathways

Id 57-11-4
Date 05.12.2003

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type : fugacity model level III
Media :
Air : % (Fugacity Model Level I)
Water : % (Fugacity Model Level I)
Soil : % (Fugacity Model Level I)
Biota : % (Fugacity Model Level II/III)
Soil : % (Fugacity Model Level II/III)
Method : other: modeling
Year : 2003

Method : EPI v3.11
Result : Level III Fugacity Model:

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.676	11.4	1000
Water	7.19	360	1000
Soil	28.9	360	1000
Sediment	63.3	1.44e+003	0

Persistence Time: 640 hr

Source : Epona Associates, LLC
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
04.12.2003

3.3.2 DISTRIBUTION

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Type : aerobic
Inoculum : activated sludge
Contact time :
Degradation : = 77 - (±) % after 28 day(s)
Result : readily biodegradable
Kinetic of testsubst. : 10 day(s) = 65 - %
14 day(s) = 69 - %
28 day(s) = 77 - %
- %
- %

Deg. product :
Method : other: BOD test
Year : 1983
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Remark : Results are an average of 11 participating laboratories.

3. Environmental Fate and Pathways

Id 57-11-4

Date 05.12.2003

Result : 65, 69 and 77 % degradation after 10, 14 and 28 days, respectively.
Source : Epona Associates, LLC
Reliability : (2) valid with restrictions
Information taken from a peer-reviewed publication.

05.12.2003

(7)

Type : aerobic
Inoculum : activated sludge
Concentration : 100 g/l related to Test substance
related to
Contact time : 5 day(s)
Degradation : - (\pm) % after
Result : readily biodegradable
Deg. product :
Method : other: BOD5
Year : 1985
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Result : Rate: .0088 1/HR

Half-Life [Days]: 3.3

Source : Epona Associates, LLC
Test condition : BOD test conducted at 20 deg C.
Reliability : (2) valid with restrictions
Information taken from a peer-reviewed publication.

05.12.2003

(14)

Type : aerobic
Inoculum : other: sewage sludge
Contact time : 21 day(s)
Degradation : = 95 - (\pm) % after 21 day(s)
Result : readily biodegradable
Deg. product :
Method : other: Sturm CO2 evolution
Year : 1984
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Source : Epona Associates, LLC
Reliability : (2) valid with restrictions
Information taken from a peer-reviewed publication.
Flag : Critical study for SIDS endpoint

05.12.2003

(13)

Type : aerobic
Inoculum : activated sludge
Contact time :
Degradation : - (\pm) % after
Result : readily biodegradable
Deg. product :
Method : other: Warburg
Year : 1973
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Result : Rate: .0077; .0052; .00217

Rate Units: 1/HR

Half-Life [Days]: 3.75; 5.55; 10.7

Source : Epona Associates, LLC

3. Environmental Fate and Pathways

Id 57-11-4
Date 05.12.2003

Test condition : Test Method: WARBURG
Oxygen Condition: AEROBIC
Analysis Method: O₂ UPTAKE
Inoculum: ACTIVATED SLUDGE
Reliability : Temperature [°C]: 20; 25; 30
(2) valid with restrictions
Information taken from a peer-reviewed publication.
05.12.2003 (11)

3.6 BOD₅, COD OR BOD₅/COD RATIO

3.7 BIOACCUMULATION

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type : static
Species : Oncorhynchus kisutch (Fish, fresh water, marine)
Exposure period : 96 hour(s)
Unit : µg/l
LC50 : = 12000 - measured/nominal
Method :
Year : 1977
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Source : Epona Associates, LLC
Test substance : "pure"
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
05.12.2003

(8)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4. Ecotoxicity

Id 57-11-4
Date 05.12.2003

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION**5.1.1 ACUTE ORAL TOXICITY**

Type : LD50
Value : = 4600 - mg/kg bw
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Doses :
Method :
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Source : Epona Associates, LLC
Reliability : (2) valid with restrictions
Information taken from a peer-reviewed publication.

05.12.2003

(2)

Type : LD100
Value : = 14286 - mg/kg bw
Species : human
Strain :
Sex :
Number of animals :
Vehicle :
Doses :
Method :
Year : 1976
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Result : Minimum/Potential Fatal Human Dose:
1. 1= PRACTICALLY NONTOXIC: PROBABLE ORAL LETHAL DOSE
(HUMAN) MORE THAN 1
QT (2.2 LB) FOR 70 KG PERSON (150 LB).

Source : Epona Associates, LLC
Reliability : (2) valid with restrictions
Information taken from a peer-reviewed publication.

05.12.2003

(4)

5.1.2 ACUTE INHALATION TOXICITY**5.1.3 ACUTE DERMAL TOXICITY****5.1.4 ACUTE TOXICITY, OTHER ROUTES**

5. Toxicity

Id 57-11-4

Date 05.12.2003

5.2.1 SKIN IRRITATION

5.2.2 EYE IRRITATION

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

Type : Sub-chronic
Species : rat
Sex :
Strain :
Route of admin. : oral feed
Exposure period : 24 weeks
Frequency of treatm. :
Post exposure period :
Doses : 50g/kg/day
Control group :
Method :
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Result : Rats fed 50 g/kg/day stearic acid for 24 weeks developed reversible lipogranulomas in adipose tissue. No significant pathological lesions were observed in rats fed 3000 ppm stearic acid orally for about 30 weeks, but anorexia, increased mortality, and a greater incidence of pulmonary infection were observed. Stearic acid is one of the least effective fatty acids in producing hyperlipemia, but the most potent in diminishing blood clotting time.

Source : Epona Associates, LLC
Reliability : (2) valid with restrictions
Information taken from a peer-reviewed publication.

05.12.2003

(2)

Type : Sub-acute
Species : rat
Sex :
Strain :
Route of admin. : oral feed
Exposure period : 6 or 9 weeks
Frequency of treatm. :
Post exposure period :
Doses : 5 or 6%
Control group :

Result : Rats fed 5% stearic acid as part of a high-fat diet for 6 weeks, or 6% stearic acid for 9 weeks, showed a decreased blood clotting time and hyperlipemia.

Source : Epona Associates, LLC
Reliability : (2) valid with restrictions
Information taken from a peer-reviewed publication.

05.12.2003

Type : Sub-acute
Species : mouse

5. Toxicity

Id 57-11-4

Date 05.12.2003

Sex :
Strain :
Route of admin. : oral feed
Exposure period : 3 weeks
Frequency of treatm. :
Post exposure period :
Doses : 5 to 50%
Control group :
Method :
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Result : When diets containing 5 to 50% stearic acid (as the monoglyceride) were fed to weanling mice for 3 weeks, depression of weight gain was seen above the 10% dietary level. Mortality occurred only with the 50% diet. The effects were less noticeable in adult mice.

Source : Epona Associates, LLC
Reliability : (2) valid with restrictions
Information taken from a peer-reviewed publication.

05.12.2003

(2)

5.5 GENETIC TOXICITY 'IN VITRO'

5.6 GENETIC TOXICITY 'IN VIVO'

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7. Eff. Against Target Org. and Intended Uses

Id 57-11-4
Date 05.12.2003

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS HANDLING AND STORING

8.2 FIRE GUIDANCE

8.3 EMERGENCY MEASURES

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

8.5 WASTE MANAGEMENT

8.6 SIDE-EFFECTS DETECTION

8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

-
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9. References

Id 57-11-4
Date 05.12.2003

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10. Summary and Evaluation

Id 57-11-4
Date 05.12.2003

10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT

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APPENDIX B
STEARIC ACID ROBUST SUMMARIES

6/8/2004

I U C L I D

Data Set

Existing Chemical	: ID: 7446-70-0
CAS No.	: 7446-70-0
EINECS Name	: aluminium chloride
EC No.	: 231-208-1
TSCA Name	: Aluminum chloride (AlCl ₃)
Molecular Formula	: AlCl ₃

Producer related part	
Company	: Epona Associates, LLC
Creation date	: 28.11.2003

Substance related part	
Company	: Epona Associates, LLC
Creation date	: 28.11.2003

Status	:
Memo	: MCC

Printing date	: 04.12.2003
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Number of pages	: 18
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Chapter (profile)	: Chapter: 2.1, 2.2, 2.4, 2.5, 2.6.1, 3.1.1, 3.1.2, 3.3.1, 3.5, 4.1, 4.2, 4.3, 5.1.1, 5.1.2, 5.1.3, 5.1.4, 5.4, 5.5, 5.6, 5.8.1, 5.8.2
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Reliability (profile)	: Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	: Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

2.1 MELTING POINT

Value : = 190 - °C
Sublimation :
Method :
Year : 1969
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Source : Epona Associates, LLC
Reliability : (2) valid with restrictions
Information taken from a peer-reviewed publication.

Flag : Critical study for SIDS endpoint
28.11.2003 (28)

2.2 BOILING POINT

Value : = 182 - °C at 1002
Decomposition :
Method :
Year : 1969
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Source : Epona Associates, LLC
Reliability : (2) valid with restrictions
Information taken from a peer-reviewed publication.

Flag : Critical study for SIDS endpoint
28.11.2003 (28)

2.4 VAPOUR PRESSURE

Value : = 1.38 - hPa at 100 °C
Decomposition :
Method :
Year : 1969
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Source : Epona Associates, LLC
Reliability : (2) valid with restrictions
Information taken from a peer-reviewed publication.

Flag : Critical study for SIDS endpoint
28.11.2003 (28)

2.5 PARTITION COEFFICIENT

Partition coefficient : octanol-water
Log pow : = 1.26 - at °C
pH value : -
Method : other (calculated)
Year : 2003
GLP : no
Test substance : as prescribed by 1.1 - 1.4

2. Physico-Chemical Data

Id 7446-70-0
Date 04.12.2003

Method : Modeled data; estimated using KOWWIN v 1.67
Source : Epona Associates, LLC
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
04.12.2003

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in : Water
Value : = 450 - g/l at 20 °C
pH value : = 2.4 -
concentration : 100 g/l at 20 °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description :
Stable :
Deg. product :
Method :
Year : 1988
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Source : BASF AG Ludwigshafen
Reliability : (4) not assignable
Original study not reviewed.
Flag : Critical study for SIDS endpoint
04.12.2003

(3)

3. Environmental Fate and Pathways

Id 7446-70-0
Date 04.12.2003

3.1.1 PHOTODEGRADATION

Type : air
Light source :
Light spectrum : - nm
Relative intensity : - based on intensity of sunlight
Deg. product :
Method :
Year : 2003
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Method : Estimated using AopWin v1.91
Result : Atmospheric Oxidation (25 deg C) [AopWin v1.91]:
Hydroxyl Radicals Reaction:
OVERALL OH Rate Constant = 0.0000 E-12 cm³/molecule-sec
Half-Life = -----
Ozone Reaction:
No Ozone Reaction Estimation

Source : Epona Associates, LLC
Reliability : (2) valid with restrictions
04.12.2003

3.1.2 STABILITY IN WATER

Type : abiotic
t1/2 pH4 : - at °C
t1/2 pH7 : - at °C
t1/2 pH9 : - at °C
Deg. product :
Method :
Year : 2000
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Remark : The material is unstable in water, 700g/l @ 15 deg C.
There is an immediate violent reaction yielding HCl gas.

Source : Whyte Chemicals Ltd London
Reliability : (4) not assignable
Original study not reviewed.

04.12.2003

(12)

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type : fugacity model level III
Media :
Air : % (Fugacity Model Level I)
Water : % (Fugacity Model Level I)
Soil : % (Fugacity Model Level I)
Biota : % (Fugacity Model Level II/III)
Soil : % (Fugacity Model Level II/III)
Method : other: modeling
Year : 2003

Method : Estimated using EPI SUMMARY (v3.11)
Remark : The material will decompose 100% in the presence of water to

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Result : give aluminium oxide and HCl gas (ECB IULCID, 2000).
: Level III Fugacity Model:
Mass Amount Half-Life Emissions
(percent) (hr) (kg/hr)
Air 5.39e-006 1e+005 1000
Water 39.8 360 1000
Soil 60.1 360 1000
Sediment 0.0767 1.44e+003 0
Persistence Time: 431 hr
Source : Epona Associates, LLC
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
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3.5 BIODEGRADATION

Deg. product :
Method : other: modeling
Year : 2003
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Remark : The material decompose 100% in the presence of water to give
aluminium oxide and HCl gas (ECB IUCLID, 2000).
Result : Probability of Rapid Biodegradation (BIOWIN v4.01):
Linear Model : 0.6841
Non-Linear Model : 0.7531
Expert Survey Biodegradation Results:
Ultimate Survey Model: 2.9045 (weeks)
Primary Survey Model : 3.6554 (days-weeks)
Readily Biodegradable Probability (MITI Model):
Linear Model : 0.3155
Non-Linear Model : 0.2102
Source : Epona Associates, LLC
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
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4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type :
Species : Brachydanio rerio (Fish, fresh water)
Exposure period : 48 hour(s)
Unit : mg/l
LC50 : = 80 -
Method :
Year : 1985
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Source : Epona Associates, LLC
Reliability : (2) valid with restrictions
28.11.2003

(9)

Type :
Species : Gambusia affinis (Fish, fresh water)
Exposure period : 24 hour(s)
Unit : mg/l
LC50 : = 29.6 - calculated
Method : other
Year : 1957
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Remark : EC50 value calculated by AQUIRE staff based on data in paper
Source : Epona Associates, LLC
Test condition : Water Parameters:
Temperature: 20 (min. value); 21 (max. value) C
Alkalinity (mg/l CaCO₃): <100 (mean value) mg/L CaCO₃ (
pH 4.3 (min. value); 7.2 (max. value)

Reliability : (2) valid with restrictions
Information taken from a peer-reviewed publication.
28.11.2003

(27)

Type :
Species : Oncorhynchus mykiss (Fish, fresh water)
Exposure period : 96 hour(s)
Unit : mg/l
LC50 : = 8.6 -

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(8)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type : static
Species : other: Ceriodaphnia dubia
Exposure period : 48 hour(s)
Unit : mg/l
EC50 : = 1.5 - measured/nominal
Method :
Year : 1986
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

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Test condition	: Water Parameters: Temperature (TMP): 25.3 (mean value); Units: C Dissolved O2 (mg/l or % saturation) (DO2): 7.3 (mean value) mg/L pH: 7.86 (mean value)	
Test substance	: 99.8% purity	
Reliability	: (2) valid with restrictions Information taken from a peer-reviewed publication.	
Flag 28.11.2003	: Critical study for SIDS endpoint	(18)
Type	: static	
Species	: Daphnia magna (Crustacea)	
Exposure period	: 48 hour(s)	
Unit	: mg/l	
EC50	: = 3.9 - calculated	
Method	:	
Year	: 1972	
GLP	: no data	
Test substance	: as prescribed by 1.1 - 1.4	
Source	: Epona Associates, LLC	
Test condition	: Water Parameters: Temperature : 18 (mean value) C Hardness(mg/l CaCO3): 45.3 (mean value)mg/L CaCO3 Alkalinity (mg/l CaCO3): 42.3 (mean value)mg/L CaCO3 Dissolved O2 (mg/l or % saturation) : 9 (mean value)mg/L pH : 7.74 (mean value)	
Reliability 28.11.2003	: (2) valid with restrictions Information taken from a peer-reviewed publication.	(5)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species	: Chlorella vulgaris (Algae)	
Endpoint	: other: popu;ation growth	
Exposure period	:	
Unit	: mg/l	
Method	:	
Year	: 2000	
GLP	:	
Test substance	: as prescribed by 1.1 - 1.4	
Result	: Effect = .225 mg/L	
Source	: BASF AG Ludwigshafen as cited in ECB IUCLID (2000)	
Test condition	: 4 months; room –temperature; pH 3.4; highest concentration tolerated: 0.002 g AlCl3 (0.05% w/v)	
Reliability 04.12.2003	: (4) not assignable Original study not reviewed.	

5.1.1 ACUTE ORAL TOXICITY

Type : LD50
Value : = 370 - mg/kg bw
Species : rat
Strain : Sprague-Dawley
Sex :
Number of animals :
Vehicle :
Doses :
Method :
Year : 1987
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Source : Epona Associates, LLC
Reliability : (2) valid with restrictions
Information taken from a peer-reviewed publication.

Flag : Critical study for SIDS endpoint

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(1) (15)

Type : LD50
Value : = 222 - mg/kg bw
Species : mouse
Strain : Swiss Webster
Sex :
Number of animals :
Vehicle :
Doses :
Method :
Year : 1987
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Source : Epona Associates, LLC
Reliability : (2) valid with restrictions
Information taken from a peer-reviewed publication.

28.11.2003

(1) (15)

Type : LD50
Value : = 770 - mg/kg bw
Species : mouse
Strain : other: Dobra Voda
Sex : male
Number of animals :
Vehicle :
Doses :
Method :
Year : 1966
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Source : Epona Associates, LLC
Reliability : (2) valid with restrictions
Information taken from a peer-reviewed publication.

28.11.2003

(1) (25)

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5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.4 REPEATED DOSE TOXICITY

Type	: Sub-acute
Species	: mouse
Sex	: female
Strain	: Swiss Webster
Route of admin.	: oral feed
Exposure period	: other: 5 or 7 weeks
Frequency of treatm.	:
Post exposure period	:
Doses	:
Control group	:
NOAEL	: = 195 - mg/kg bw
Method	:
Year	: 1993
GLP	: no data
Test substance	: as prescribed by 1.1 - 1.4
Remark	: Approximate feed concentrations of 250 and 350 ppm aluminum (ATSDR, 1999)
Result	: Mice that ingested doses higher than 130 mg Al/kg/day as aluminum chloride for 49 days, and were tested using a standardized neurotoxicity screening battery, also showed decreased motor activity, as well as decreased grip strength and startle responsiveness. Signs of neurotoxicity but no change in hematocrit levels, no liver changes at 195 mg/kg/day. No body weight changes at 260 mg/kg/day.
Source	: Epona Associates, LLC
Test condition	: Adult mice consumed aluminum chloride for 5-7 weeks in a diet that also contained 3.5% sodium citrate.
Reliability	: (2) valid with restrictions Information taken from a peer-reviewed publication.
28.11.2003	(1) (26)
Type	: Sub-chronic
Species	: mouse
Sex	: male/female
Strain	: other: Dobra Voda
Route of admin.	: other: drinking water and base diet
Exposure period	: up to 390 days
Frequency of treatm.	:
Post exposure period	:
Doses	: 19.3 or 49 mg/kg/day
Control group	: yes
Method	:
Year	: 1966
GLP	: no
Test substance	: as prescribed by 1.1 - 1.4
Result	: No change in lung histology and no hepatic effects when exposed to 19.3

	mg/kg/day for 390 days.
	No effects on body weight at any dose or exposure time. No hematological effects, no histological changes in the femurs of male and female Dobra Voda
	mice given 49 mg Al/kg/day as aluminum chloride in drinking water for 180 or 390 days (ATSDR, 1999). No renal effects in male or female animals given 49 mg/kg/day for 180 days or 19.3 mg/kg/day for 390 days.
	No organ weight or histological changes in the spleen or thymus and the body weights of male and female Dobra Voda mice were similar to controls following
	exposure to 49 mg Al/kg/day as aluminum chloride in drinking water and base diet for 180 or 390 days (ATSDR, 1999)
Reliability	: (2) valid with restrictions
28.11.2003	Information taken from a peer-reviewed publication. (1) (25)
28.11.2003	

5.5 GENETIC TOXICITY 'IN VITRO'

Type	: Salmonella typhimurium reverse mutation assay
System of testing	: TA102
Test concentration	: 0.3, 3 ppm (0.3, 3 mg/l)
Cycotoxic concentr.	:
Metabolic activation	:
Result	: negative
Method	: other: according to Ames, B.N. et al.: Mutat. Res. 31, 347–164
Year	: 1985
GLP	: no data
Test substance	: no data
Remark	: Preincubation test with solutions containing 0.3 and 3.0 ppm of the test substance.
Source	: BASF AG Ludwigshafen as cited in ECB IUCLID (2000) Epona Associates, LLC
Reliability	: (2) valid with restrictions
Flag	: Critical study for SIDS endpoint
04.12.2003	(1) (2) (17)
Type	: other: Rec Assay
System of testing	: Bacillus subtilis
Test concentration	:
Cycotoxic concentr.	:
Metabolic activation	:
Result	: negative
Method	:
Year	: 1980
GLP	: no data
Test substance	: no data
Source	: Epona Associates, LLC
Reliability	: (2) valid with restrictions
28.11.2003	(1) (14)
Type	: other: Thymidine incorporation
System of testing	: rat osteoblasts
Test concentration	:
Cycotoxic concentr.	:
Metabolic activation	:

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Result	:		
Method	:		
Year	:	1989	
GLP	:	no data	
Test substance	:		
Remark	:	"aluminum may impede cell cycle progression. Generalizations to normal, untransformed cells, however, cannot be made." (ATSDR, 1999)	
Source	:	Epona Associates, LLC	
Reliability	:	(2) valid with restrictions	(1) (6)
28.11.2003			
Type	:	Mammalian cell gene mutation assay	
System of testing	:	Syrian hamster embryo cells	
Test concentration	:		
Cycotoxic concentr.	:		
Metabolic activation	:		
Result	:	negative	
Method	:		
Year	:	1979	
GLP	:	no data	
Test substance	:	no data	
Source	:	Epona Associates, LLC	
Reliability	:	(2) valid with restrictions Information taken from a peer-reviewed publication.	(1) (10)
28.11.2003			
Type	:	other: DNA cross-linking	
System of testing	:	Rat ascites hepatoma cells	
Test concentration	:	500 umol/l	
Cycotoxic concentr.	:		
Metabolic activation	:		
Result	:	positive	
Method	:		
Year	:	1986	
GLP	:	no data	
Test substance	:	no data	
Remark	:	"Cross-linking agents frequently produce clastogenic effects due, presumably, to conformational distortions that prohibit proper DNA replication." (ATSDR, 1999)	
Source	:	Epona Associates, LLC	
Reliability	:	(2) valid with restrictions Information taken from a peer-reviewed publication.	(1) (29)
28.11.2003			
Type	:	Ames test	
System of testing	:	Salmonella typhimurium TA1537 TA2637 TA98 TA100 TA102	
Test concentration	:		
Cycotoxic concentr.	:		
Metabolic activation	:		
Result	:	negative	
Method	:		
Year	:	1987	
GLP	:	no data	
Test substance	:	as prescribed by 1.1 - 1.4	
Source	:	BASF AG Ludwigshafen as cited in ECB IUCLID (2000)	
Reliability	:	(4) not assignable	(24)
04.12.2003			

5. Toxicity

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Type : Mouse lymphoma assay
System of testing : L5178Y TK+/- Mouse Lymphoma cells
Test concentration : 570, 580, 590, 600, 620, 625 ug/ml
Cycotoxic concentr. :
Metabolic activation : with and without
Result : negative
Method : other: according to Clive, D. et al.: Mutat. Res. 59, 61-108
Year : 1979
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Remark : forward mutation assay with and without metabolic activation with S9-mix prepared from liver homogenate of Aroclor pretreated Sprague-Dawley rats; the mutation frequency remained constant at ca. 2-fold

Source : BASF AG Ludwigshafen as cited in ECB IUCLID (2000)
Test substance : aluminium chloride; according to the authors, the compound was of certified ACS grade

Reliability : (4) not assignable
Original study not reviewed.

04.12.2003

(22) (23)

5.6 GENETIC TOXICITY 'IN VIVO'

Type : Micronucleus assay
Species : mouse
Sex :
Strain :
Route of admin. : i.p.
Exposure period : bone marrow cells were fixed at times up to 72 h
Doses : .01, .05 or .1 molar aluminum chloride
Result : positive
Method :
Year : 1972
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Result : "There was a significant increase in chromatid-type aberrations over the controls, and these occurred in a nonrandom distribution over the chromosome complement. No dose-response relationship could be demonstrated, although the highest dose of aluminum chloride did produce the greatest number of aberrations." (ATSDR, 1999)
The effect was qualitatively more or less the same at different intervals as well as at different concentrations in the form of erosion, stickiness, etc. as general and subchromatid, chromatid and chromosome breaks, translocations, gaps and constrictions in the individual chromosomes.

Source : BASF AG Ludwigshafen as cited in ECB IUCLID (2000)
Epona Associates, LLC

Test condition : Mice were injected intraperitoneally with 0.01, 0.05, or 0.1 molar aluminum chloride, and bone marrow cells were examined for chromosomal aberrations.

Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint

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(1) (16)

5.8.1 TOXICITY TO FERTILITY

Type : Fertility
Species : rat
Sex :
Strain : Sprague-Dawley
Route of admin. : drinking water
Exposure period : up to 90 d prior to breeding
Frequency of treatm. :
Premating exposure period
 Male : 90 days
 Female :
Duration of test : 160 days
No. of generation studies :
Doses : 0; 5; 50; 500 mg/l (Al-equivalent) = 0; 44.8; 447.6; 4476.0 mg/l (AlCl₃)
Control group : yes, concurrent no treatment
Method :
Year : 1979
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Remark : AlCl₃ was tested as AlCl₃ · 6H₂O; molecular weight 241 and aluminium equivalent weight of 11%.
Result : No abnormalities in the reproductive capacity of the males measured by histopathologic evaluation, plasma gonadotropin level and serial mating of the males to untreated virgin females over a 70 d posttreatment breeding period.
Source : BASF AG Ludwigshafen as cited in ECB IUCLID (2000)
Reliability : (4) not assignable
 Original study not reviewed.

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(11)

Type : other: three generation
Species : mouse
Sex :
Strain : Swiss Webster
Route of admin. : other: drinking water and base diet
Exposure period : 180 - 390 d (weanlings were treated from 4. week of age like parents) 390 days

Frequency of treatm. :
Premating exposure period
 Male :
 Female :
Duration of test :
No. of generation studies : 3
Doses : 0; 19.3 mg/kg/d (doses expressed in terms of Al)
Control group :
Result : no effects on fertility
Method :
Year : 1966
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Remark : "Aluminum apparently does not affect reproduction. Finally, pharmacokinetic data do not indicate that the reproductive organs are target organs" (ATSDR, 1999)
Result : There were no significant differences in the numbers of

litters or off-spring between the treated and control mice. Growth was retarded and was dependent on the intake of aluminium, but the effect did not appear in the first generation or in the first litter. The subsequent litters manifested a very marked growth retardation, as did those of the third generation. An analysis of variance established that, under the conditions of our experiment, weight variations could be accounted for by aluminium uptake ($P < 0.001$). The differences in the course of weight plots for successive generations and litters were also statistically significant ($P < 0.01$).

The erythrocyte counts and haemoglobin levels in the first and last generations did not differ significantly from those in the controls; and no pathological changes could be found in the tissues examined.

Source : BASF AG Ludwigshafen as cited in ECB IUCLID (2000)
Epona Associates, LLC
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
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(1) (25)

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

Species : rat
Sex : female
Strain : other: THA
Route of admin. : gavage
Exposure period : on day 15 of pregnancy
Frequency of treatm. : single dose
Duration of test : until 10 weeks post parturition
Doses : 900, 1800 mg/kg
Control group : yes, concurrent no treatment
Method :
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Remark : According to the authors, the doses applied in this study corresponded with ca. 1/4 and 1/2 of the acute oral LD50 of the test substance for adult rats.

Result : The effects of prenatal aluminium treatment on development and behaviour were studied. Four and three pregnant rats of the 22nd generation of the THA strain were administered the test substance dissolved in saline at doses of 900 and 1800 mg/kg, respectively; another 3 rats were given saline (control). The day of parturition was designated as postnatal day 0. Body weights of the litters were recorded on postnatal days 1, 7, 14, 21, and 28. Pups were weaned at postnatal day 21. Twenty offsprings (10 males and 10 females) each of the dams of each aluminium treated group and 10 males and 18 female offsprings of control dams were selected for behavioural tests (Sidman avoidance test on postnatal days 28 to 38; open field test at 10 weeks post partum). Statistically significant differences in body weight gain, timing of pinna detachment and eye opening, and appearances of auditory startle were observed between the aluminium treated offspring and controls. Behavioural tests revealed slower learning acquisition in the treated groups. The longer latency and more rearings in the open field test

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	were observed in the female pups of high dose group dams. According to the authors, these results suggested that a single dose of the test substance during prenatal period affected both the development and behaviour of the offspring in rats.	
Source	: BASF AG Ludwigshafen as cited in ECB IUCLID (2000)	
Test substance	: aluminium chloride; purity >98%	
Reliability	: (4) not assignable	
	Original study not reviewed.	
04.12.2003		(21)
Species	: rat	
Sex	: female	
Strain	: Sprague-Dawley	
Route of admin.	: oral feed	
Exposure period	: Gestation day 6, 9, 12, 15 and 18	
Frequency of treatm.	: continuously in the diet on treatment days	
Duration of test	: 20 days	
Doses	: 500, 1000 ppm in the diet (ca. 45, 91 mg/kg/d, respectively)	
Control group	:	
NOAEL maternal tox.	: = 110 - mg/kg bw	
Method	:	
Year	: 1979	
GLP	: no data	
Test substance	: as prescribed by 1.1 - 1.4	
Remark	: "The 110 mg Al/kg/day dose is not a definite NOAEL because the intermittent daily exposure schedule could have missed a critical developmental time for inducing effects. Concurrent administration of parathyroid hormone by subcutaneous injection, which increased tissue levels of aluminum by presumably enhancing its absorption, increased the percentage of resorbed or dead fetuses." (ATSDR, 1999)	
Result	: Comment: Normal food contained 119 ppm Al "Rats that ingested up to 110 mg Al/kg/day in feed that contained added aluminum chloride on Gd 6, 9, 12, 15, and 18 did not experience maternal toxicity, embryo/fetal toxicity, teratogenicity, fetal growth retardation, or significantly increased fetal whole carcass concentrations of aluminum " (ATSDR, 1999) Resorption rate was increased following 1000 ppm Al and Parathyroid Hormone (PTH) – subcutaneous injections of 68 units/kg on gestational days 6, 9, 12, 15, and 18 – suggesting that this metal and hormone may be embryotoxic when administered throughout organogenesis and late fetal development (day 6–19). Neither PTH nor 1000 ppm Al alone had any effect on mortality and the apparent no-effect dose level for embryotoxicity after combined treatment is 500 ppm Al and PTH.	
Source	: BASF AG Ludwigshafen as cited in ECB IUCLID (2000)	
	Epona Associates, LLC	
Reliability	: (2) valid with restrictions	
	Information taken from a peer-reviewed publication.	
Flag	: Critical study for SIDS endpoint	
04.12.2003		(1) (20)
Species	: rat	
Sex	:	
Strain	: Sprague-Dawley	
Route of admin.	: oral feed	
Exposure period	: from day 6 of gestation through day 19	

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Frequency of treatm.	: continuously in the diet	
Duration of test	: 20 days	
Doses	: 0.1 % in the diet (ca. 91 mg/kg/d)	
Control group	: no data specified	
Remark	: Maternal tox.: No effect reported	
Result	: No significant effect on dam body weight gain, fetal weight or length, resorption rate or incidence of soft tissue or skeletal anomalies.	
Source	: BASF AG Ludwigshafen as cited in ECB IUCLID (2000)	
Reliability	: (4) not assignable	
04.12.2003	Original study not reviewed.	(19)
Species	: rat	
Sex	: female	
Strain	: other: Holtzmann	
Route of admin.	: i.p.	
Exposure period	: days 9-13 or 14-18 of gestation	
Frequency of treatm.	: 5 times	
Duration of test	: 20 days	
Doses	: 0; 75; 100; 200 mg/kg (AlCl ₃ crystals solved in sterile dist. water)	
Control group	: yes, concurrent no treatment	
Remark	: Maternal tox.: – Dose dependent death in 100– and 200 mg/kg group; – Stat. sign. differences in maternal weight gain at dose level 75 and 100 (treated on days 14–18 of gestation). – In many cases maternal liver was severely damaged (perihepatic granulomas, signs of centrilobular necrosis).	
Result	: Offsprings treated with AlCl ₃ showed sign growth retardation as well as skeletal defects; incidence of fetal death and resorption was significantly increased. 75 mg/kg (day 14–18 of gestation): no malformation There was no clear dose–response relationship respect to mean weight and length of fetuses. 100 mg/kg (day 14–18 of gestation): Three fetuses (from 2 litters) had abnormal digits. 7 fetuses (from 4 litters) had wavy ribs – in cases ribs were missing. A large number of fetuses showed poor ossification (cranid bones, lower part of vertebral column, bones of limbs). 200 mg/kg: High incidence of dead offspring	
Source	: BASF AG Ludwigshafen as cited in ECB IUCLID (2000)	
Reliability	: (4) not assignable	
04.12.2003	Original study not reviewed.	(4) (13)

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APPENDIX C
ALUMNIMUM DISTEARATE ROBUST SUMMARIES

6/8/2004

I U C L I D

Data Set

Existing Chemical	: ID: 300-92-5
CAS No.	: 300-92-5
EINECS Name	: hydroxyaluminium distearate
EC No.	: 206-101-8
Molecular Formula	: C36H71AlO5

Producer related part	
Company	: Epona Associates, LLC
Creation date	: 05.12.2003

Substance related part	
Company	: Epona Associates, LLC
Creation date	: 05.12.2003

Status	:
Memo	: SOCMA MCC

Printing date	: 06.12.2003
Revision date	:
Date of last update	: 06.12.2003

Number of pages	: 14
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Chapter (profile)	: Chapter: 2.1, 2.2, 2.4, 2.5, 2.6.1, 3.1.1, 3.1.2, 3.3.1, 3.5, 4.1, 4.2, 4.3, 5.1.1, 5.1.2, 5.1.3, 5.1.4, 5.4, 5.5, 5.6, 5.8.1, 5.8.2
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Reliability (profile)	: Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	: Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

2. Physico-Chemical Data

Id 300-92-5
Date 06.12.2003

2.1 MELTING POINT

Value : = 145 - °C
Sublimation :
Method :
Year : 1987
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Source : Epona Associates, LLC
Reliability : (2) valid with restrictions
Information taken from a peer-reviewed publication.

Flag : Critical study for SIDS endpoint
05.12.2003 (2)

2.2 BOILING POINT

Remark : The boiling points of the dissociation products are: 190 deg C (aluminum chloride) and 69-70 deg C (Stearic acid).
This endpoint is not applicable due to the physical state the substance.

Source : Epona Associates, LLC
Reliability : (2) valid with restrictions
06.12.2003

2.4 VAPOUR PRESSURE

Remark : The estimated vapor pressure is 4E-17 mm Hg EPI SUMMARY (v3.11)
The vapor pressures of the dissociation products are: 1.38 @ 100 deg C (aluminum chloride) and 1.33 @ 174 deg C (Stearic acid).
This endpoint is not applicable due to the physical state the substance.

Reliability : (2) valid with restrictions
06.12.2003

2.5 PARTITION COEFFICIENT

Partition coefficient : octanol-water
Log pow : - at °C
pH value : -
Method :
Year : 2003
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Remark : Aluminum distearate is not soluble in water.
The partition coefficients of the dissociation products are: 1.26 (calculated) (aluminum chloride) and 8.42 (Stearic acid).

Reliability : (2) valid with restrictions
06.12.2003

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

2. Physico-Chemical Data

Id 300-92-5

Date 06.12.2003

Solubility in	:	Water
Value	:	- at °C
pH value	:	-
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	not soluble
Stable	:	
Deg. product	:	
Method	:	
Year	:	2003
GLP	:	
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Water Solubility Estimate from Log Kow (WSKOW v1.41) Water Solubility at 25 deg C (mg/L): 1.776e-011 Aluminum distearate is not soluble in water. The water solubilities of the dissociation products are: 450 @ 20 deg C (aluminum chloride) and .00568 @ 25 deg C (Stearic acid).
Source	:	Epona Associates, LLC
Reliability	:	(2) valid with restrictions

06.12.2003

3. Environmental Fate and Pathways

Id 300-92-5
Date 06.12.2003

3.1.1 PHOTODEGRADATION

Type : air
Light source :
Light spectrum : - nm
Relative intensity : - based on intensity of sunlight
DIRECT PHOTOLYSIS
Half-life t_{1/2} : = .2 - day(s)
Degradation : - % after
Quantum yield :
INDIRECT PHOTOLYSIS
Sensitizer :
Conc. of sensitizer :
Rate constant : = .000000000043 cm³/(molecule*sec)
Degradation : - % after
Deg. product :
Method :
Year : 2003
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Result : Atmospheric Oxidation (25 deg C) [AopWin v1.91]:
Hydroxyl Radicals Reaction:
OVERALL OH Rate Constant = 43.0498 E-12 cm³/molecule-sec
Half-Life = 0.248 Days (12-hr day; 1.5E6 OH/cm³)
Half-Life = 2.981 Hrs
Ozone Reaction:
No Ozone Reaction Estimation
Source : Epona Associates, LLC
Reliability : (2) valid with restrictions
06.12.2003 (1)

3.1.2 STABILITY IN WATER

Deg. product :
Method :
Year : 2003
GLP :
Test substance : as prescribed by 1.1 - 1.4

Remark : Aluminum distearate is not soluble in water.
The hydrolysis data for the dissociation products is: "unstable" (aluminum chloride) and not available due to low water solubility (stearic acid)
Source : Epona Associates, LLC
Reliability : (2) valid with restrictions
06.12.2003

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type : fugacity model level III
Media :
Air : % (Fugacity Model Level I)
Water : % (Fugacity Model Level I)
Soil : % (Fugacity Model Level I)
Biota : % (Fugacity Model Level II/III)
Soil : % (Fugacity Model Level II/III)

Id 300-92-5
Date 06.12.2003

3.5 BIODEGRADATION

5 / 5

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Method :
Year : 2003
GLP :
Test substance : as prescribed by 1.1 - 1.4

Remark : Aluminum distearate is not soluble in water, and is expected to readily dissociate to Aluminum and Stearic acid.
Species: Oncorhynchus mykiss (Fish, fresh water)
Exposure period 96 hour(s)
Unit: mg/l
LC50: = 8.6
Test Substance: Aluminum chloride
Reference: Call, DJ, LT Brooke, CA Lindberg, TP Markee, DJ MaCauley, and SH Poirier (1984) Toxicity of Aluminum to Freshwater Organisms in Water of pH 6.5-8.5. Tech Rep Project No. 549-238-RT-WRD, Center for Lake Superior Environmental Studies, University of Wisconsin, Superior, WI. /November 27, 1984 Memo to C Stephan, USEPA, Duluth, MN:46 p (Author Communication Used).

Type:static
Species: Oncorhynchus kisutch (Fish, fresh water, marine)
Exposure period: 96 hour(s)
Unit: µg/l
LC50: = 12000 - measured/nominal
Method:
Year: 1977
GLP: no data
Test substance: Stearic acid

Test substance: "pure"
Reliability: (2) valid with restrictions
Flag: Critical study for SIDS endpoint
Reference: SIDS Leach, J.M. and A.N. Thakore (1977)
Compounds Toxic to Fish Pulp Mill Waste Streams Progress in Water Technology, 9: 787-798 CIS Record ID.: AQ-0132049

Source : Epona Associates, LLC
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
06.12.2003

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Method :
Year : 2003
GLP :
Test substance : as prescribed by 1.1 - 1.4

Remark : Acute toxicity to aquatic invertebrates was not located for stearic acid.
Aluminum distearate is not soluble in water, and is expected to readily dissociate to Aluminum and Stearic acid.
Type:static
Species other: Ceriodaphnia dubia
Exposure period : 48 hour(s)
Unit: mg/l
EC50: = 1.5 - measured/nominal

Method:
Year: 1986
GLP: no data
Test substance: as prescribed by 1.1 - 1.4

Test condition: Water Parameters:
Temperature (TMP): 25.3 (mean value); Units: C
Dissolved O2 (mg/l or % saturation) (DO2): 7.3 (mean value) mg/L
pH: 7.86 (mean value)

Test substance: Aluminum chloride, 99.8% purity
Reliability: (2) valid with restrictions
Information taken from a peer-reviewed publication.

Flag: Critical study for SIDS endpoint
Reference: McCauley, D.J., L.T. BROOKE, D.J. CALL and C.A.
LINDBERG (1986) Acute and Chronic Toxicity of Aluminum to
Ceriodaphnia dubia at Various pH's. Center for Lake Superior
Environmental Studies, University of Wisconsin, Superior, WI: 15; 1986
CIS Record ID.: AQ-0113175

Source : Epona Associates, LLC
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
06.12.2003

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Remark : Acute toxicity to aquatic invertebrates or aquatic plants was not located for stearic acid or aluminum chloride.
Aluminum distearate is not soluble in water, and is expected to readily dissociate to Aluminum and Stearic acid.

Source : Epona Associates, LLC
Reliability : (2) valid with restrictions
06.12.2003

5.1.1 ACUTE ORAL TOXICITY

Method :
Year : 2003
GLP :
Test substance : other TS: Dissociation products

Remark : Aluminum distearate is expected to readily dissociate to Aluminum and Stearic acid.
Type: LD50
Value: = 370 - mg/kg bw
Species: rat
Strain: Sprague-Dawley
Year: 1987
GLP: no data
Test substance: Aluminum chloride
Reliability: (2) valid with restrictions
Information taken from a peer-reviewed publication.
Flag: Critical study for SIDS endpoint
Reference: Agency for Toxic Substances and Disease Registry [ATSDR] 1999, Toxicological Profile for Aluminum; and Llobet JM, Domingo JL, Gomez M, et al. 1987. Acute toxicity studies of aluminum compounds: Antidotal efficacy of several chelating agents. Pharmacol Toxicol 60:280-283. Llobet et al (1987)

Type: LD50
Value: = 4600 - mg/kg bw
Species: rat
GLP: no data
Test substance: stearic acid
Reliability: (2) valid with restrictions
Information taken from a peer-reviewed publication.
Reference: Clayton, G.D., F.E. Clayton (eds.) Patty's Industrial Hygiene and Toxicology. Volumes 2A, 2B, 2C, 2D, 2E, 2F: Toxicology. 4th ed. New York, NY: John Wiley & Sons Inc., 1993-1994. 3568. Cited in BiblioLine

Source : Epona Associates, LLC
Reliability : (2) valid with restrictions
06.12.2003

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.4 REPEATED DOSE TOXICITY

Method :
Year : 2003
GLP :
Test substance : other TS: Dissociation products

Remark : Aluminum distearate is expected to readily dissociate to Aluminum and

Stearic acid.
 Type: Sub-acute
 Species: mouse
 Sex: female
 Strain: Swiss Webster
 Route of admin.: oral feed
 Exposure period: other: 5 or 7 weeks
 NOAEL: = 195 - mg/kg bw
 Year: 1993
 GLP: no data
 Test substance: Aluminum chloride

Remark: Approximate feed concentrations of 250 and 350 ppm aluminum (ATSDR, 1999)
 Result: Mice that ingested doses higher than 130 mg Al/kg/day as aluminum chloride for 49 days, and were tested using a standardized neurotoxicity screening battery, also showed decreased motor activity, as well as decreased grip strength and startle responsiveness.
 Signs of neurotoxicity but no change in hematocrit levels, no liver changes at 195 mg/kg/day. No body weight changes at 260 mg/kg/day.
 Test condition: Adult mice consumed aluminum chloride for 5-7 weeks in a diet that also contained 3.5% sodium citrate.
 Reliability: (2) valid with restrictions
 Information taken from a peer-reviewed publication.
 Reference: Agency for Toxic Substances and Disease Registry [ATSDR] 1999, Toxicological Profile for Aluminum; and Oteiza PI, Keen CL, Han B, et al. 1993. Aluminum accumulation and neurotoxicity in Swiss-mice after long-term dietary exposure to aluminum and citrate. Metabolism 42:1296-1300.

Type: Sub-chronic
 Species: rat
 Route of admin.: oral feed
 Exposure period: 24 weeks
 Doses: 50g/kg/day
 GLP: no data
 Test substance: Stearic acid

Result: Rats fed 50 g/kg/day stearic acid for 24 weeks developed reversible lipogranulomas in adipose tissue. No significant pathological lesions were observed in rats fed 3000 ppm stearic acid orally for about 30 weeks, but anorexia, increased mortality, and a greater incidence of pulmonary infection were observed. Stearic acid is one of the least effective fatty acids in producing hyperlipemia, but the most potent in diminishing blood clotting time.
 Reliability: (2) valid with restrictions
 Information taken from a peer-reviewed publication.

Reference: Clayton, G.D., F.E. Clayton (eds.) Patty's Industrial Hygiene and Toxicology. Volumes 2A, 2B, 2C, 2D, 2E, 2F: Toxicology. 4th ed. New York, NY: John Wiley & Sons Inc., 1993-1994. 3568. Cited in BiblioLine

Source : Epona Associates, LLC
 Reliability : (2) valid with restrictions
 Flag : Critical study for SIDS endpoint
 06.12.2003

5.5 GENETIC TOXICITY 'IN VITRO'

Type :

5. Toxicity

Id 300-92-5
Date 06.12.2003

System of testing	:	
Test concentration	:	
Cycotoxic concentr.	:	
Metabolic activation	:	
Result	:	
Method	:	
Year	:	2003
GLP	:	
Test substance	:	other TS: Dissociation products
Remark	:	<p>Aluminum distearate is expected to readily dissociate to Aluminum and Stearic acid. Genotoxicity data were not located for Stearic Acid. Multiple studies with bacterial systems indicate aluminum chloride is not a bacterial mutagen. This is one of several studies summarized in the Aluminum chloride IUCLID. Type: Ames test System of testing: Salmonella typhimurium TA1537 TA2637 TA98 TA100 TA102 Test concentration: Result: negative Year: 1987 GLP: no data Test substance: Aluminum chloride Source: BASF AG Ludwigshafen as cited in ECB IUCLID (2000) Reliability: (4) not assignable Reference: Ogawa H.I. et al.: Jpn.J.Genet. 62, 159-162, (1987)</p> <p>Multiple studies with in vitro mammalian systems indicate aluminum chloride is not genotoxic. This is one of several studies summarized in the Aluminum chloride IUCLID.</p> <p>Type: Mouse lymphoma assay System of testing: L5178Y TK+/- Mouse Lymphoma cells Test concentration: 570, 580, 590, 600, 620, 625 ug/ml Metabolic activation: with and without Result: negative Method: other: according to Clive, D. et al.: Mutat. Res. 59, 61-108 Year: 1979 GLP: no data Test substance: Aluminum chloride Remark: forward mutation assay with and without metabolic activation with S9-mix prepared from liver homogenate of Aroclor pretreated Sprague-Dawley rats; the mutation frequency remained constant at ca. 2-fold Source: BASF AG Ludwigshafen as cited in ECB IUCLID (2000) Test substance: aluminium chloride; according to the authors, the compound was of certified ACS grade Reliability: (4) not assignable Original study not reviewed. Reference: Oberly T.J. and Piper C.E.: Environ. Mutag. 2, 281 (1980); abstract as cited in ECB IUCLID (2000); and Oberly T.J. et al.: J. Toxicol. Environ. Health 9, 367-376 (1982) as cited in ECB IUCLID (2000)</p>
Source	:	Epona Associates, LLC
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint
06.12.2003		

5.6 GENETIC TOXICITY 'IN VIVO'

5. Toxicity

Id 300-92-5

Date 06.12.2003

Type	:	
Species	:	
Sex	:	
Strain	:	
Route of admin.	:	
Exposure period	:	
Doses	:	
Result	:	
Method	:	
Year	:	2003
GLP	:	
Test substance	:	other TS: Dissociation products
Remark	:	<p>Aluminum distearate is expected to readily dissociate to Aluminum and Stearic acid. Genotoxicity data were not located for Stearic Acid. Type: Micronucleus assay Species: mouse Route of admin.: i.p. Exposure period : bone marrow cells were fixed at times up to 72 h Doses: .01, .05 or .1 molar aluminum chloride Result: positive Year: 1972 GLP: no data Test substance: Aluminum chloride Result: "There was a significant increase in chromatid-type aberrations over the controls, and these occurred in a nonrandom distribution over the chromosome complement. No dose-response relationship could be demonstrated, although the highest dose of aluminum chloride did produce the greatest number of aberrations." (ATSDR, 1999) The effect was qualitatively more or less the same at different intervals as well as at different concentrations in the form of erosion, stickiness, etc. as general and subchromatid, chromatid and chromosome breaks, ranslocations, gaps and constrictions in the individual chromosomes. Source: BASF AG Ludwigshafen as cited in ECB IUCLID (2000) Epona Associates, LLC Test condition: Mice were injected intraperitoneally with 0.01, 0.05, or 0.1 molar aluminum chloride, and bone marrow cells were examined for chromosomal aberrations. Reliability: (2) valid with restrictions Flag: Critical study for SIDS endpoints. Reference: Agency for Toxic Substances and Disease Registry [ATSDR] 1999, Toxicological Profile for Aluminum; and Manna GK, Das RK. 1972. Chromosome aberrations in mice induced by aluminum chloride. Nucleus 15:180-186.</p>
Source	:	Epona Associates, LLC
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

06.12.2003

5.8.1 TOXICITY TO FERTILITY

Method	:	
Year	:	2003

GLP	:	
Test substance	:	other TS: Dissociation products
Remark	:	<p>Aluminum distearate is expected to readily dissociate to Aluminum and Stearic acid.</p> <p>Effects on fertility data were not located for Stearic Acid.</p> <p>Type: other: three generation</p> <p>Species: mouse</p> <p>Strain: Swiss Webster</p> <p>Route of admin.: other: drinking water and base diet</p> <p>Exposure period: 180 - 390 d (weanlings were treated from 4. week of age like parents) 390 days</p> <p>No. of generation studies: 3</p> <p>Doses: 0; 19.3 mg/kg/d (doses expressed in terms of Al)</p> <p>Result: no effects on fertility</p> <p>Year: 1966</p> <p>GLP: no data</p> <p>Test substance: Aluminum chloride</p> <p>Remark: "Aluminum apparently does not affect reproduction. Finally, pharmacokinetic data do not indicate that the reproductive organs are target organs" (ATSDR, 1999)</p> <p>Result: There were no significant differences in the numbers of litters or offspring between the treated and control mice. Growth was retarded and was dependent on the intake of aluminium, but the effect did not appear in the first generation or in the first litter. The subsequent litters manifested a very marked growth retardation, as did those of the third generation. An analysis of variance established that, under the conditions of our experiment, weight variations could be accounted for by aluminium uptake ($P < 0.001$). The differences in the course of weight plots for successive generations and litters were also statistically significant ($P < 0.01$).</p> <p>The erythrocyte counts and haemoglobin levels in the first and last generations did not differ significantly from those in the controls; and no pathological changes could be found in the tissues examined.</p> <p>Source: BASF AG Ludwigshafen as cited in ECB IUCLID (2000)</p> <p>Reliability: (2) valid with restrictions</p> <p>Reference: Agency for Toxic Substances and Disease Registry [ATSDR] 1999, Toxicological Profile for Aluminum; and Ondreicka R, Ginter E, Kortus J. 1966. Chronic toxicity of aluminum in rats and mice and its effects on phosphorus metabolism Br J Ind Med 23:305-312.</p>
Source	:	Epona Associates, LLC
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint
06.12.2003		

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

Method	:	
Year	:	2003
GLP	:	
Test substance	:	other TS: Dissociation products
Remark	:	<p>Aluminum distearate is expected to readily dissociate to Aluminum and Stearic acid.</p> <p>Developmental effects data were not located for Stearic Acid.</p> <p>Species: rat</p>

Sex: female
Strain: other: Holtzmann
Route of admin.: i.p.
Exposure period: days 9-13 or 14-18 of gestation
Frequency of treatm.: 5 times
Duration of test: 20 days
Doses: 0; 75; 100; 200 mg/kg (AlCl₃ crystals solved in sterile dist.water)
Control group: yes, concurrent no treatment
Remark: Maternal tox.:
- Dose dependent death in 100- and 200 mg/kg group;
- Stat. sign. differences in maternal weight gain at dose level 75 and 100 (treated on days 14-18 of gestation).
- In many cases maternal liver was severely damaged (perihepatic granulomas, signs of centrilobular necrosis).
Result: Offsprings treated with AlCl₃ showed sign growth retardation as well as skeletal defects; incidence of fetal death and resorption was significantly increased.
75 mg/kg (day 14-18 of gestation): no malformation
There was no clear dose-response relationship respect to mean weight and length of fetuses.
100 mg/kg (day 14-18 of gestation): Three fetuses (from 2 litters) had abnormal digits.
7 fetuses (from 4 litters) had wavy ribs - in cases ribs were missing.
A large number of fetuses showed poor ossification (cranid bones, lower part of vertebral column, bones of limbs).
200 mg/kg: High incidence of dead offspring
Test Substance: aluminum chloride
Source: BASF AG Ludwigshafen as cited in ECB IUCLID (2000)
Reliability: (4) not assignable
Reference: Benett R.W. et al.: Anat.Anz. 138, 365-378, (1975) as cited in ECB IUCLID (2000)igElinder C.-G. and Sjoegren B. in: Friberg L.(Ed.) et al.: Handbook on the Toxicology Metals, 2nd. Ed., 1-25, Elsevier, (1986) as cited in ECB IUCLID (2000)

Source
Reliability
Flag
06.12.2003

: Epona Associates, LLC
: (2) valid with restrictions
: Critical study for SIDS endpoint

- (1) EPIWIN v 3.11
- (2) Sax, N.I. and R.J. Lewis, Sr. (eds.). Hawley's Condensed Chemical Dictionary. 11th ed. New York: Van Nostrand Reinhold Co., 1987.
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APPENDIX D
ALUMNIMUM TRISTEARATE ROBUST SUMMARIES

6/8/2004

I U C L I D

Data Set

Existing Chemical	: ID: 637-12-7
CAS No.	: 637-12-7
EINECS Name	: aluminium tristearate
EC No.	: 211-279-5
Molecular Formula	: C ₁₈ H ₃₆ O ₂ .1/3Al

Producer related part	
Company	: Epona Associates, LLC
Creation date	: 06.12.2003

Substance related part	
Company	: Epona Associates, LLC
Creation date	: 06.12.2003

Status	:
Memo	: SOCMA MCC

Printing date	: 07.12.2003
Revision date	:
Date of last update	: 07.12.2003

Number of pages	: 15
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Chapter (profile)	: Chapter: 2.1, 2.2, 2.4, 2.5, 2.6.1, 3.1.1, 3.1.2, 3.3.1, 3.5, 4.1, 4.2, 4.3, 5.1.1, 5.1.2, 5.1.3, 5.1.4, 5.4, 5.5, 5.6, 5.8.1, 5.8.2
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Reliability (profile)	: Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	: Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

2. Physico-Chemical Data

Id 637-12-7
Date 07.12.2003

2.1 MELTING POINT

Value : = 100 - 120 °C
Sublimation :
Method :
Year : 2002
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Test substance : Purity = 100%
Reliability : (2) valid with restrictions

06.12.2003

(3)

Value : = 117 - 120 °C
Sublimation :
Method :
Year : 2003
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Source : Epona Associates, LLC
Reliability : (2) valid with restrictions
Information taken from a peer-reviewed source.
Flag : Critical study for SIDS endpoint

06.12.2003

(7)

2.2 BOILING POINT

Decomposition : yes
Method :
Year : 2003
GLP :
Test substance : as prescribed by 1.1 - 1.4

Source : Epona Associates, LLC
Test substance : Purity = 100%
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint

06.12.2003

(3)

2.4 VAPOUR PRESSURE

Decomposition :
Method : other (calculated)
Year : 2002
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Result : 1.08E-018 mm Hg (Modified Grain method)
Source : Epona Associates, LLC
Reliability : (3) invalid
Flag : Critical study for SIDS endpoint

06.12.2003

(4)

2. Physico-Chemical Data

Id 637-12-7
Date 07.12.2003

2.5 PARTITION COEFFICIENT

Partition coefficient : octanol-water
Log pow : = 22.69 - at °C
pH value : -
Method : other (calculated)
Year : 2003
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Remark : Aluminum tristearate is expected to dissociate to aluminum and stearic acid.
Source : Epona Associates, LLC
Reliability : (3) invalid
Endpoint not applicable as the material is not soluble in water.
Flag : Critical study for SIDS endpoint
06.12.2003 (2)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in : Water
Value : - at °C
pH value : -
concentration : at °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description : not soluble
Stable :
Deg. product :
Method :
Year : 1983
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Source : Epona Associates, LLC
Reliability : (2) valid with restrictions
Information taken from a peer-reviewed source.
06.12.2003 (6)

Solubility in : Water
Value : - at °C
pH value : -
concentration : at °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description :
Stable :
Deg. product :
Method : other: calculated
Year : 2003
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Result : Water Solubility Estimate from Log Kow (WSKOW v1.41):
Water Solubility at 25 deg C (mg/L): 9.386e-020
Source : Epona Associates, LLC
Reliability : (3) invalid

2. Physico-Chemical Data

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Endpoint not applicable as the material is not soluble in water.

(2)

3. Environmental Fate and Pathways

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3.1.1 PHOTODEGRADATION

Type : air
Light source :
Light spectrum : - nm
Relative intensity : - based on intensity of sunlight
DIRECT PHOTOLYSIS
Half-life t_{1/2} : = .2 - day(s)
Degradation : - % after
Quantum yield :
INDIRECT PHOTOLYSIS
Sensitizer :
Conc. of sensitizer :
Rate constant : = .000000000064 cm³/(molecule*sec)
Degradation : - % after
Deg. product :
Method : other (calculated)
Year : 2003
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Result : Atmospheric Oxidation (25 deg C) [AopWin v1.91]:
Hydroxyl Radicals Reaction:
OVERALL OH Rate Constant = 64.3647 E-12 cm³/molecule-sec
Half-Life = 0.166 Days (12-hr day; 1.5E6 OH/cm³)
Half-Life = 1.994 Hrs
Ozone Reaction:
No Ozone Reaction Estimation
Source : Epona Associates, LLC
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint

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(2)

3.1.2 STABILITY IN WATER

Deg. product :
Method :
Year : 2003
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Remark : Aluminum tristearate is not soluble in water.
The hydrolysis data for the dissociation products is: "unstable" (aluminum chloride) and not available due to low water solubility (stearic acid)
Source : Epona Associates, LLC
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint

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3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type : fugacity model level III
Media :
Air : % (Fugacity Model Level I)
Water : % (Fugacity Model Level I)
Soil : % (Fugacity Model Level I)

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Biota : % (Fugacity Model Level II/III)
Soil : % (Fugacity Model Level II/III)
Method : other: estimated
Year : 2003

Result : Level III Fugacity Model:
Mass Amount Half-Life Emissions
(percent) (hr) (kg/hr)
Air 0.0598 3.99 1000
Water 2.35 1.44e+003 1000
Soil 29.9 1.44e+003 1000
Sediment 67.7 5.76e+003 0
Persistence Time: 2.61e+003 hr

Source : Epona Associates, LLC
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
06.12.2003 (2)

3.5 BIODEGRADATION

Deg. product :
Method : other: calculated
Year : 2003
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Remark : Aluminum tristearate is not soluble in water.
The biodegradation of the dissociation products are: not applicable -
unstable in water (aluminum chloride) and readily biodegradable (Stearic
acid).

Result : Probability of Rapid Biodegradation (BIOWIN v4.01):
Linear Model : 0.6551
Non-Linear Model : 0.0195
Expert Survey Biodegradation Results:
Ultimate Survey Model: 2.1552 (months)
Primary Survey Model: 3.3890 (days -weeks)
Readily Biodegradable Probability (MITI Model):
Linear Model : 0.4750
Non-Linear Model : 0.1062

Source : Epona Associates, LLC
Reliability : (3) invalid
Endpoint not applicable as the material is not soluble in water.
07.12.2003 (2)

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Method :
Year : 2003
GLP :
Test substance : other TS: Dissociation products

Remark : Aluminum tristearate is not soluble in water, and is expected to readily dissociate to Aluminum and Stearic acid.
Species: Oncorhynchus mykiss (Fish, fresh water)
Exposure period 96 hour(s)
Unit: mg/l
LC50: = 8.6
Test Substance: Aluminum chloride
Reference: Call, DJ, LT Brooke, CA Lindberg, TP Markee, DJ MaCauley, and SH Poirier (1984) Toxicity of Aluminum to Freshwater Organisms in Water of pH 6.5-8.5. Tech Rep Project No. 549-238-RT-WRD, Center for Lake Superior Environmental Studies, University of Wisconsin, Superior, WI. /November 27, 1984 Memo to C Stephan, USEPA, Duluth, MN:46 p (Author Communication Used).

Type: static
Species: Oncorhynchus kisutch (Fish, fresh water, marine)
Exposure period: 96 hour(s)
Unit: µg/l
LC50: = 12000 - measured/nominal
Method:
Year: 1977
GLP: no data
Test substance: Stearic acid

Test substance: "pure"
Reliability: (2) valid with restrictions
Flag: Critical study for SIDS endpoint
Reference: SIDS Leach, J.M. and A.N. Thakore (1977)
Compounds Toxic to Fish Pulp Mill Waste Streams Progress in Water Technology, 9: 787-798 CIS Record ID.: AQ-0132049

Source : Epona Associates, LLC
Reliability : (2) valid with restrictions
07.12.2003

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Method :
Year : 2003
GLP :
Test substance : other TS: Dissociation products

Remark : Acute toxicity to aquatic invertebrates was not located for stearic acid.
Aluminum tristearate is not soluble in water, and is expected to readily dissociate to Aluminum and Stearic acid.
Type: static
Species other: Ceriodaphnia dubia
Exposure period : 48 hour(s)
Unit: mg/l
EC50: = 1.5 - measured/nominal
Method:

Year: 1986
GLP: no data
Test substance: as prescribed by 1.1 - 1.4

Test condition: Water Parameters:
Temperature (TMP): 25.3 (mean value); Units: C
Dissolved O2 (mg/l or % saturation) (DO2): 7.3 (mean value) mg/L
pH: 7.86 (mean value)

Test substance: Aluminum chloride, 99.8% purity
Reliability: (2) valid with restrictions
Information taken from a peer-reviewed publication.

Flag: Critical study for SIDS endpoint
Reference: McCauley, D.J., L.T. BROOKE, D.J. CALL and C.A.
LINDBERG (1986) Acute and Chronic Toxicity of Aluminum to
Ceriodaphnia dubia at Various pH's. Center for Lake Superior
Environmental Studies, University of Wisconsin, Superior, WI: 15; 1986
CIS Record ID.: AQ-0113175

Source : Epona Associates, LLC
Reliability : (2) valid with restrictions
07.12.2003

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Method :
Year : 2003
GLP :
Test substance : other TS: Dissociation products

Remark : Acute toxicity to aquatic invertebrates or aquatic plants was not located for
stearic acid or aluminum chloride.
Aluminum distearate is not soluble in water, and is expected to readily
dissociate to Aluminum and Stearic acid.

Reliability : (2) valid with restrictions
07.12.2003

5.1.1 ACUTE ORAL TOXICITY

Method :
Year : 2003
GLP :
Test substance : other TS: Dissociation products

Remark : Aluminum tristearate is expected to readily dissociate to Aluminum and Stearic acid.
Type: LD50
Value: = 370 - mg/kg bw
Species: rat
Strain: Sprague-Dawley
Year: 1987
GLP: no data
Test substance: Aluminum chloride
Reliability: (2) valid with restrictions
Information taken from a peer-reviewed publication.
Flag: Critical study for SIDS endpoint
Reference: Agency for Toxic Substances and Disease Registry [ATSDR] 1999, Toxicological Profile for Alumunim; and Llobet JM, Domingo JL, Gomez M, et al. 1987. Acute toxicity studies of aluminum compounds: Antidotal efficacy of several chelating agents. Pharmacol Toxicol 60:280-283.Llobet et al (1987)

Type: LD50
Value: = 4600- mg/kg bw
Species: rat
GLP: no data
Test substance: stearic acid
Reliability: (2) valid with restrictions
Information taken from a peer-reviewed publication.
Reference: Clayton, G.D., F.E. Clayton (eds.) Patty's Industrial Hygiene and Toxicology. Volumes 2A, 2B, 2C, 2D, 2E, 2F: Toxicology. 4th ed. New York, NY: John Wiley & Sons Inc., 1993-1994. 3568. Cited in BiblioLine

Source : Epona Associates, LLC
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
07.12.2003

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.4 REPEATED DOSE TOXICITY

Method :
Year : 2003
GLP :
Test substance : other TS: Dissociation products

Remark	: Aluminum tristearate is expected to readily dissociate to Aluminum and Stearic acid. Type: Sub-acute Species: mouse Sex: female Strain: Swiss Webster Route of admin.: oral feed Exposure period: other: 5 or 7 weeks NOAEL: = 195 - mg/kg bw Year: 1993 GLP: no data Test substance: Aluminum chloride
	Remark: Approximate feed concentrations of 250 and 350 ppm aluminum (ATSDR, 1999) Result: Mice that ingested doses higher than 130 mg Al/kg/day as aluminum chloride for 49 days, and were tested using a standardized neurotoxicity screening battery, also showed decreased motor activity, as well as decreased grip strength and startle responsiveness. Signs of neurotoxicity but no change in hematocrit levels, no liver changes at 195 mg/kg/day. No body weight changes at 260 mg/kg/day. Test condition: Adult mice consumed aluminum chloride for 5-7 weeks in a diet that also contained 3.5% sodium citrate. Reliability: (2) valid with restrictions Information taken from a peer-reviewed publication. Reference: Agency for Toxic Substances and Disease Registry [ATSDR] 1999, Toxicological Profile for Aluminum; and Oteiza PI, Keen CL, Han B, et al. 1993. Aluminum accumulation and neurotoxicity in Swiss-mice after long-term dietary exposure to aluminum and citrate. Metabolism 42:1296-1300.
	Type: Sub-chronic Species: rat Route of admin.: oral feed Exposure period: 24 weeks Doses: 50g/kg/day GLP: no data Test substance: Stearic acid
	Result: Rats fed 50 g/kg/day stearic acid for 24 weeks developed reversible lipogranulomas in adipose tissue. No significant pathological lesions were observed in rats fed 3000 ppm stearic acid orally for about 30 weeks, but anorexia, increased mortality, and a greater incidence of pulmonary infection were observed. Stearic acid is one of the least effective fatty acids in producing hyperlipemia, but the most potent in diminishing blood clotting time. Reliability: (2) valid with restrictions Information taken from a peer-reviewed publication. Reference: Clayton, G.D., F.E. Clayton (eds.) Patty's Industrial Hygiene and Toxicology. Volumes 2A, 2B, 2C, 2D, 2E, 2F: Toxicology. 4th ed. New York, NY: John Wiley & Sons Inc., 1993-1994. 3568. Cited in BibliLine
Source	: Epona Associates, LLC
Reliability	: (2) valid with restrictions
Flag	: Critical study for SIDS endpoint
07.12.2003	

5. Toxicity

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Type	:	
System of testing	:	
Test concentration	:	
Cycotoxic concentr.	:	
Metabolic activation	:	
Result	:	
Method	:	
Year	:	2003
GLP	:	
Test substance	:	other TS: Dissociatin products
Remark	:	<p>Aluminum tristearate is expected to readily dissociate to Aluminum and Stearic acid.</p> <p>Genotoxicity data were not located for Stearic Acid.</p> <p>Multiple studies with bacterial systems indicate aluminum chloride is not a bacterial mutagen. This is one of several studies summarized in the Aluminum chloride IUCLID.</p> <p>Type: Ames test</p> <p>System of testing: Salmonella typhimurium TA1537 TA2637 TA98 TA100 TA102</p> <p>Test concentration:</p> <p>Result: negative</p> <p>Year: 1987</p> <p>GLP: no data</p> <p>Test substance: Aluminum chloride</p> <p>Source: BASF AG Ludwigshafen as cited in ECB IUCLID (2000)</p> <p>Reliability: (4) not assignable</p> <p>Reference: Ogawa H.I. et al.: Jpn.J.Genet. 62, 159-162, (1987)</p> <p>Multiple studies with in vitro mammalian systems indicate aluminum chloride is not genotoxic. This is one of several studies summarized in the Aluminum chloride IUCLID.</p> <p>Type: Mouse lymphoma assay</p> <p>System of testing: L5178Y TK+/- Mouse Lymphoma cells</p> <p>Test concentration: 570, 580, 590, 600, 620, 625 ug/ml</p> <p>Metabolic activation: with and without</p> <p>Result: negative</p> <p>Method: other: according to Clive, D. et al.: Mutat. Res. 59, 61-108</p> <p>Year: 1979</p> <p>GLP: no data</p> <p>Test substance: Aluminum chloride</p> <p>Remark: forward mutation assay with and without metabolic activation with S9-mix prepared from liver homogenate of Aroclor pretreated Sprague-Dawley rats; the mutation frequency remained constant at ca. 2-fold</p> <p>Source: BASF AG Ludwigshafen as cited in ECB IUCLID (2000)</p> <p>Test substance: aluminium chloride; according to the authors, the compound was of certified ACS grade</p> <p>Reliability: (4) not assignable</p> <p>Original study not reviewed.</p> <p>Reference: Oberly T.J. and Piper C.E.: Environ. Mutag. 2, 281 (1980); abstract as cited in ECB IUCLID (2000); and Oberly T.J. et al.: J. Toxicol. Environ. Health 9, 367-376 (1982) as cited in ECB IUCLID (2000)</p>
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint
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5.6 GENETIC TOXICITY 'IN VIVO'

5. Toxicity

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Type	:	
Species	:	
Sex	:	
Strain	:	
Route of admin.	:	
Exposure period	:	
Doses	:	
Result	:	
Method	:	
Year	:	2003
GLP	:	
Test substance	:	other TS: Dissociation products
Remark	:	<p>Aluminum tristearate is expected to readily dissociate to Aluminum and Stearic acid. Genotoxicity data were not located for Stearic Acid. Type: Micronucleus assay Species: mouse Route of admin.: i.p. Exposure period : bone marrow cells were fixed at times up to 72 h Doses: .01, .05 or .1 molar aluminum chloride Result: positive Year: 1972 GLP: no data Test substance: Aluminum chloride Result: "There was a significant increase in chromatid-type aberrations over the controls, and these occurred in a nonrandom distribution over the chromosome complement. No dose-response relationship could be demonstrated, although the highest dose of aluminum chloride did produce the greatest number of aberrations." (ATSDR, 1999) The effect was qualitatively more or less the same at different intervals as well as at different concentrations in the form of erosion, stickiness, etc. as general and subchromatid, chromatid and chromosome breaks, ranslocations, gaps and constrictions in the individual chromosomes. Source: BASF AG Ludwigshafen as cited in ECB IUCLID (2000) Epona Associates, LLC Test condition: Mice were injected intraperitoneally with 0.01, 0.05, or 0.1 molar aluminum chloride, and bone marrow cells were examined for chromosomal aberrations. Reliability: (2) valid with restrictions Flag: Critical study for SIDS endpoints. Reference: Agency for Toxic Substances and Disease Registry [ATSDR] 1999, Toxicological Profile for Aluminum; and Manna GK, Das RK. 1972. Chromosome aberrations in mice induced by aluminum chloride. Nucleus 15:180-186.</p>
Source	:	Epona Associates, LLC
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

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5.8.1 TOXICITY TO FERTILITY

Method	:	
Year	:	2003
GLP	:	

Test substance	: other TS: Dissociation products
Remark	<p>: Aluminum tristearate is expected to readily dissociate to Aluminum and Stearic acid.</p> <p>Effects on fertility data were not located for Stearic Acid.</p> <p>Type: other: three generation</p> <p>Species: mouse</p> <p>Strain: Swiss Webster</p> <p>Route of admin.: other: drinking water and base diet</p> <p>Exposure period: 180 - 390 d (weanlings were treated from 4. week of age like parents) 390 days</p> <p>No. of generation studies: 3</p> <p>Doses: 0; 19.3 mg/kg/d (doses expressed in terms of Al)</p> <p>Result: no effects on fertility</p> <p>Year: 1966</p> <p>GLP: no data</p> <p>Test substance: Aluminum chloride</p> <p>Remark: "Aluminum apparently does not affect reproduction. Finally, pharmacokinetic data do not indicate that the reproductive organs are target organs" (ATSDR, 1999)</p> <p>Result: There were no significant differences in the numbers of litters or offspring between the treated and control mice. Growth was retarded and was dependent on the intake of aluminium, but the effect did not appear in the first generation or in the first litter. The subsequent litters manifested a very marked growth retardation, as did those of the third generation. An analysis of variance established that, under the conditions of our experiment, weight variations could be accounted for by aluminium uptake ($P < 0.001$). The differences in the course of weight plots for successive generations and litters were also statistically significant ($P < 0.01$).</p> <p>The erythrocyte counts and haemoglobin levels in the first and last generations did not differ significantly from those in the controls; and no pathological changes could be found in the tissues examined.</p> <p>Source: BASF AG Ludwigshafen as cited in ECB IUCLID (2000)</p> <p>Reliability: (2) valid with restrictions</p> <p>Reference: Agency for Toxic Substances and Disease Registry [ATSDR] 1999, Toxicological Profile for Aluminum; and Ondreicka R, Ginter E, Kortus J. 1966. Chronic toxicity of aluminum in rats and mice and its effects on phosphorus metabolism Br J Ind Med 23:305-312.</p>
Source	: Epona Associates, LLC
Reliability	: (2) valid with restrictions
Flag	: Critical study for SIDS endpoint
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5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

Method	:
Year	: 2003
GLP	:
Test substance	: other TS: Dissociation products
Remark	<p>: Aluminum tristearate is expected to readily dissociate to Aluminum and Stearic acid.</p> <p>Developmental effects data were not located for Stearic Acid.</p> <p>Species: rat</p> <p>Sex: female</p> <p>Strain: other: Holtzmann</p>

Route of admin.: i.p.
Exposure period: days 9-13 or 14-18 of gestation
Frequency of treatm.: 5 times
Duration of test: 20 days
Doses: 0; 75; 100; 200 mg/kg (AlCl₃ crystals solved in sterile dist.water)
Control group: yes, concurrent no treatment
Remark: Maternal tox.:
- Dose dependent death in 100- and 200 mg/kg group;
- Stat. sign. differences in maternal weight gain at dose level 75 and 100 (treated on days 14-18 of gestation).
- In many cases maternal liver was severely damaged (perihepatic granulomas, signs of centrilobular necrosis).
Result: Offsprings treated with AlCl₃ showed sign growth retardation as well as skeletal defects; incidence of fetal death and resorption was significantly increased.
75 mg/kg (day 14-18 of gestation): no malformation
There was no clear dose-response relationship respect to mean weight and length of fetuses.
100 mg/kg (day 14-18 of gestation): Three fetuses (from 2 litters) had abnormal digits.
7 fetuses (from 4 litters) had wavy ribs - in cases ribs were missing.
A large number of fetuses showed poor ossification (cranid bones, lower part of vertebral column, bones of limbs).
200 mg/kg: High incidence of dead offspring
Test Substance: aluminum chloride
Source: BASF AG Ludwigshafen as cited in ECB IUCLID (2000)
Reliability: (4) not assignable
Reference: Benett R.W. et al.: Anat.Anz. 138, 365-378, (1975) as cited in ECB IUCLID (2000)igElinder C.-G. and Sjoegren B. in: Friberg L.(Ed.) et al.: Handbook on the Toxicology Metals, 2nd. Ed., 1-25, Elsevier, (1986) as cited in ECB IUCLID (2000)
Source : Epona Associates, LLC
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint

Source
Reliability
Flag
07.12.2003

9. References

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- (2) EPIWIN v. 3.11
- (3) Mallinckrodt Inc. (2002) Material Data Safety Sheet Aluminum Tristearate 3/13/2002
- (4) MPBPWIN v1.41
- (6) The Merck Index. 10th ed. Rahway, New Jersey: Merck Co., Inc., 1983. 54
- (7) The Merck Index. 10th ed. Rahway, New Jersey: Merck Co., Inc., 1983. 54